4-Hexylresorcinol
136-77-6 | DTXSID1020699

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.90e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.92e-01

Confidence level: 6.40e-01

Nearest Neighbors from the Training Set

Image not found
11-Hydroxyundecanoic acid
Measured: 1.98e-03
Predicted: 2.24e-03

Image not found
Terpin
Measured: 2.06e-02
Predicted: 3.89e-02

Image not found
Terpin
Measured: 2.06e-02
Predicted: 3.89e-02

Image not found
2,2-Bis(bromomethyl)-1,3-
propanediol
Measured: 1.45e-01
Predicted: 2.34e-01